

08.897,455

Page 1

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L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

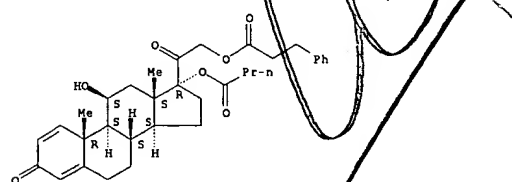
ACCESSION NUMBER: 1995:648143 CAPLUS  
 DOCUMENT NUMBER: 123:56394  
 TITLE: Corticoid 17,21-dicarboxylates and 17-carboxylate-21-carbonates as topical inflammation inhibitors  
 INVENTOR(S): Stache, Ulrich; Alpermann, Hans-Georg; Duerckheimer, Walter; Bohn, Manfred  
 PATENT ASSIGNEE(S): Hoechst A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 45 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 646593	A1	19950405	EP 1994-115348	19940929
EP 646593	B1	20011205		
DE 4333920	A1	19950413	DE 1993-4333920	19931005
AT 210143	Z	20011215	AT 1994-115348	19940929
ES 2168283	TJ	20020616	ES 1994-115348	19940929
CN 1108661	A	19950920	CN 1994-116479	19940930
CN 1051316	B	20000412		
FI 9404599	A	19950406	FI 1994-4599	19941003
AU 9474395	A1	19950427	AU 1994-74395	19941003
AU 679551	B2	19970703		
HU 68577	A2	19950628	HU 1994-2831	19941003
HU 219401	B	20010428		
IL 111132	A1	20001031	IL 1994-111132	19941003
CA 2133607	AA	19950406	CA 1994-2133607	19941004
NO 9403701	A	19950406	NO 1994-3701	19941004
ZA 9407739	A	19950518	ZA 1994-7739	19941004
JP 07165788	A2	19950627	JP 1994-263234	19941004
US 2002103392	A1	20020801	US 1997-897455	19970722
PRIORITY APPLN. INFO.:			DE 1993-4333920 A	19931005
			US 1994-310791 B1	19940929
			US 1996-590624 B1	19960124

OTHER SOURCE(S): MARPAT 123:56394  
 AB Title eters I [A = CHOH, CHCl, CH<sub>2</sub>, CO; AY = bond; Y = H, F, Cl; Z = H, F, Me; R1 = (un)substituted alkyl, aryl, heteroaryl; R2 = alkyl, Ph, CH<sub>2</sub>Ph; R3 = H, Me; n = 0, 1] were prep. from the 17-monoesters. Thus prednisolone 17-benzoate was treated with PhCH<sub>2</sub>CO<sub>2</sub>H and dicyclohexylcarbodiimide and pyridinium sulfate in pyridine to give the 21-phenylacetate (II). At 1.0 mg/ml, applied topically with croton oil, II gave 91% inhibition of the croton oil edema in rats.  
 IT 164343-59-3P 164344-01-8P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (corticoid 17,21-dicarboxylates and 17-carboxylate-21-carbonates as topical inflammation inhibitors)  
 RN 164343-59-3 CAPLUS  
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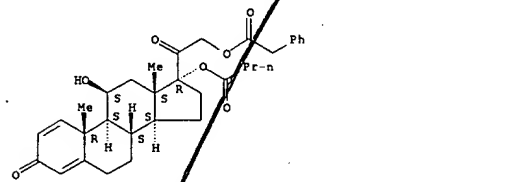
L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Absolute stereochemistry.



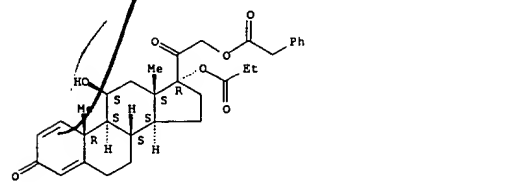
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Absolute stereochemistry.



RN 164343-57-1 CAPLUS  
 CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-17-(1-oxopropoxy)-21-[(phenylacetyl)oxy]-, (11.beta.)- (9CI) (CA INDEX NAME)

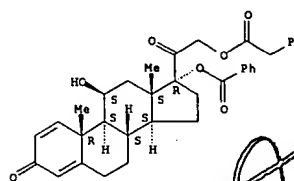
Absolute stereochemistry.



RN 164343-58-2 CAPLUS

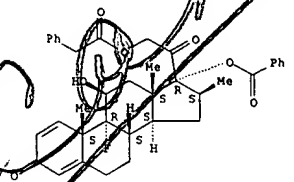
L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Absolute stereochemistry.



RN 164344-01-8 CAPLUS  
 CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-17-(1-oxobutoxy)-9-fluoro-11-hydroxy-16-methyl-21-[(phenylacetyl)oxy]-, (11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 164343-43-5P 164343-56-0P 164343-57-1P  
 164343-58-2P 164343-60-6P 164343-61-7P  
 164343-64-0P 164343-70-8P 164343-74-2P  
 164343-75-3P 164343-76-4P 164343-77-5P  
 164343-78-6P 164343-79-7P 164343-80-0P  
 164343-81-1P 164343-82-2P 164343-83-3P  
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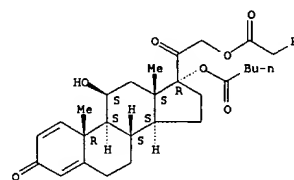
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (corticoid 17,21-dicarboxylates and 17-carboxylate-21-carbonates as topical inflammation inhibitors)

RN 164343-43-5 CAPLUS  
 CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-17-(1-oxobutoxy)-21-(1-oxo-3-phenylpropoxy)-, (11.beta.)- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

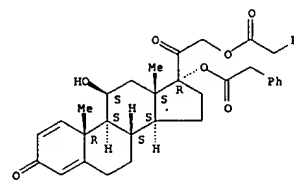
CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-17-(1-oxopentyl)oxy)-21-[(phenylacetyl)oxy]-, (11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 164343-60-6 CAPLUS  
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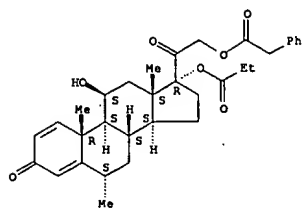
Absolute stereochemistry.



RN 164343-61-7 CAPLUS  
 CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-6-methyl-17-(1-oxopropoxy)-21-[(phenylacetyl)oxy]-, (6.alpha.,11.beta.)- (9CI) (CA INDEX NAME)

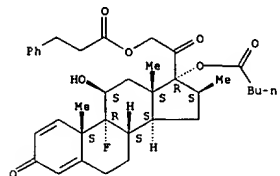
Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 164343-64-0 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17-[(1-oxopentyl)oxy]-21-[(1-oxo-3-phenylpropoxy)]-, (11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

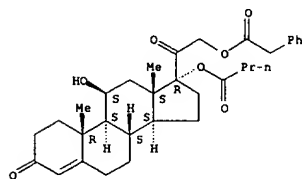
Absolute stereochemistry.



RN 164343-70-8 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17-[(1-oxopentyl)oxy]-21-[(phenylacetyl)oxy]-, (11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

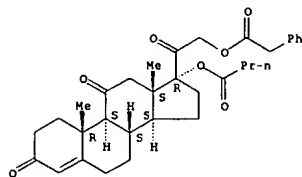
Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



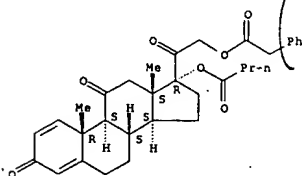
RN 164343-76-4 CAPLUS  
CN Pregna-1,4-diene-3,11,20-trione, 17-[(1-oxobutoxy)-21-[(phenylacetyl)oxy]]-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.



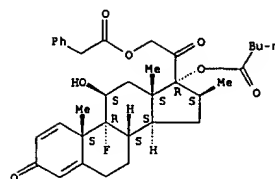
RN 164343-77-5 CAPLUS  
CN Pregna-1,4-diene-3,11,20-trione, 17-[(1-oxobutoxy)-21-[(phenylacetyl)oxy]]-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.



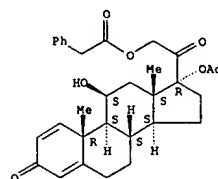
RN 164343-78-6 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 6-fluoro-11-hydroxy-17-[(1-oxobutoxy)-21-[(phenylacetyl)oxy]]-, (6.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 164343-74-2 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 17-(acetyloxy)-11-hydroxy-21-[(phenylacetyl)oxy]-, (11.beta.)- (9CI) (CA INDEX NAME)

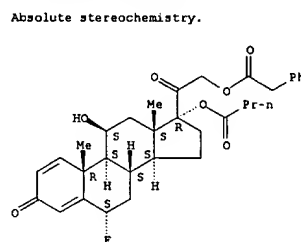
Absolute stereochemistry.



RN 164343-75-3 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-17-[(1-oxobutoxy)-21-[(phenylacetyl)oxy]]-, (11.beta.)- (9CI) (CA INDEX NAME)

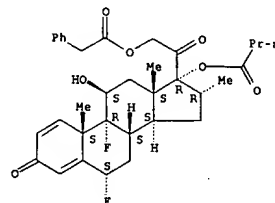
Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 164343-79-7 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 6,9-difluoro-11-hydroxy-16-methyl-17-[(1-oxobutoxy)-21-[(phenylacetyl)oxy]]-, (6.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

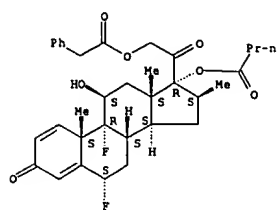
Absolute stereochemistry.



RN 164343-80-0 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 6,9-difluoro-11-hydroxy-16-methyl-17-[(1-oxobutoxy)-21-[(phenylacetyl)oxy]]-, (6.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

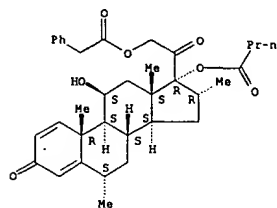
Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 164343-81-1 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 11-hydroxy-6,16-dimethyl-17-(1-oxobutoxy)-21-[(phenylacetyl)oxy]-, (6.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

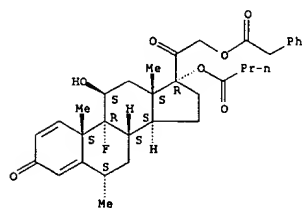
Absolute stereochemistry.



RN 164343-82-2 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 17-(1-oxobutoxy)-21-[(phenylacetyl)oxy]- (9CI) (CA INDEX NAME)

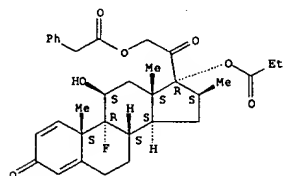
Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



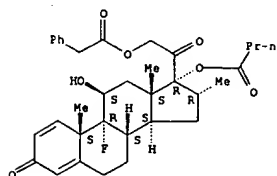
RN 164343-85-5 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17-(1-oxopropoxy)-21-[(phenylacetyl)oxy]-, (11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

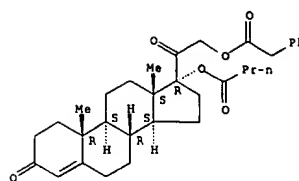


RN 164343-86-6 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17-(1-oxobutoxy)-21-[(phenylacetyl)oxy]-, (11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

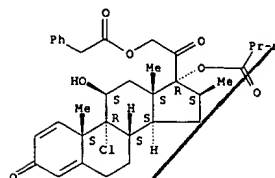


L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 164343-83-3 CAPLUS  
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Absolute stereochemistry.



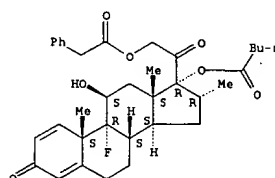
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CN Pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17-(1-oxobutoxy)-21-[(phenylacetyl)oxy]-, (6.alpha.,11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

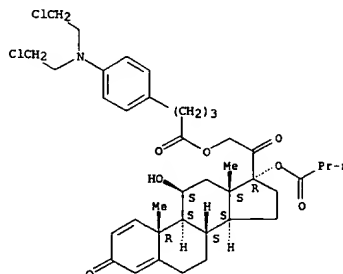
RN 164343-87-7 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17-[(1-oxopentyl)oxy]-21-[(phenylacetyl)oxy]-, (11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 164343-88-8 CAPLUS  
CN Pregna-1,4-diene-3,20-dione, 21-[4-{4-[bis(2-chloroethyl)amino]phenyl}-1-oxobutoxy]-11-hydroxy-17-(1-oxobutoxy)-, (11.beta.)- (9CI) (CA INDEX NAME)

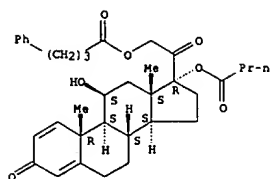
Absolute stereochemistry.



RN 164344-08-5 CAPLUS  
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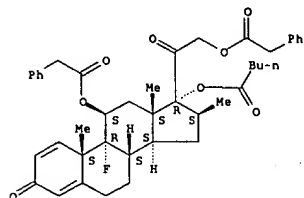
Absolute stereochemistry.

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 164344-36-9 CAPLUS  
 CN Pregn-4-ene-3,20-dione, 9-fluoro-16-methyl-17-[(1-oxopentyl)oxy]-11,21-bis[(phenylacetyl)oxy]-, (11.β.,16.β.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

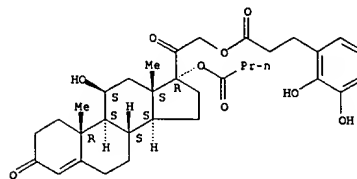
ACCESSION NUMBER: 1973:515784 CAPLUS  
 DOCUMENT NUMBER: 79:115784  
 TITLE: Corticosteroid 17- and 21-esters  
 INVENTOR(S): Yarrow, Hyman; Whitefield, Martin; Little, John H.  
 PATENT ASSIGNEE(S): Dermal Laboratories Ltd.  
 SOURCE: Ger. Offen., 28 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2204366	A1	19730802	DE 1972-2204366	19720127
PRIORITY APPLN. INFO.:		DE 1972-2204366 19720127		

AB Hydrocortisone and prednisolone 17- and 21-esters (10 compds.), useful as anti-inflammatory agents, were prepd. Thus, hydrocortisone was esterified with PrC(OEt)3 to yield I (RR1 = CPrOEt) which was converted to I (R = H, R1 = PrCO). Mesylation of I (R = H, R1 = PrCO) followed by treatment with NaI yielded iodopregnenedione II, which was esterified with 2,3-(HO)2-C6H3(CH2)2CO2H to give I (R = 2,3-(HO)2C6H3(CH2)2CO).

IT 49756-90-3P 49756-91-4P 49756-92-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 49756-90-3 CAPLUS  
 CN Pregn-4-ene-3,20-dione, 21-[3-(2,3-dihydroxyphenyl)-1-oxopropoxy]-11-hydroxy-17-(1-oxobutoxy)-, (11.β.)- (9CI) (CA INDEX NAME)

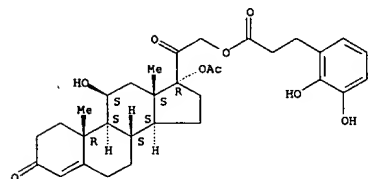
Absolute stereochemistry.



RN 49756-91-4 CAPLUS  
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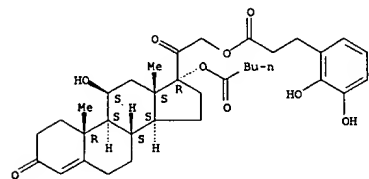
Absolute stereochemistry.

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 49756-92-5 CAPLUS  
 CN Pregn-4-ene-3,20-dione, 21-[3-(2,3-dihydroxyphenyl)-1-oxopropoxy]-11-hydroxy-17-[(1-oxopentyl)oxy]-, (11.β.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 12:04:52 ON 01 MAR 2004)

FILE 'REGISTRY' ENTERED AT 12:05:08 ON 01 MAR 2004

L1 STRUCTURE UPLOADED

L2 5 S L1

L3 118 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:06:11 ON 01 MAR 2004

L4 142 S L3

L5 70 S L4 NOT PY>=1992

FILE 'REGISTRY' ENTERED AT 12:08:51 ON 01 MAR 2004

L6 STRUCTURE UPLOADED

L7 57 S L6 FULL SUB=L3

L8 STRUCTURE UPLOADED

L9 30 S L8 FULL SUB=L3

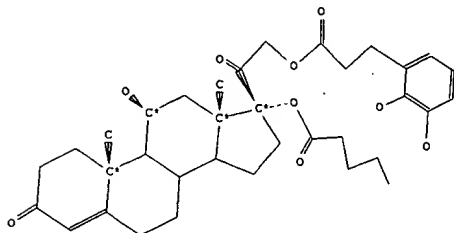
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L10 2 S L9

=> d all 1-3

## L11 ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2932013  
 Beilstein Pref. RN (BPR): 49756-92-5  
 CAS Reg. No. (RN): 49756-92-5  
 Chemical Name (CN): Hydrocortison-17-valerat-21-<.beta.->(2,3-dihydroxyphenyl)-propionat  
 Autonom Name (AUN): pentanoic acid 17-<<3-(2,3-dihydroxyphenyl)-propionyloxy>-acetyl>-11-hydroxy-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta<a>phenanthren-17-yl ester  
 Molec. Formula (MF): C35 H46 O9  
 Molecular Weight (MW): 610.74  
 Lawson Number (LN): 12033, 10058, 1182  
 File Segment (FS): Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 2718794  
 Tautomer ID (TAUTID): 2888485  
 Beilstein Citation (BSO): 5-10  
 Entry Date (DED): 1989/07/11  
 Update Date (DUPD): 1989/07/26

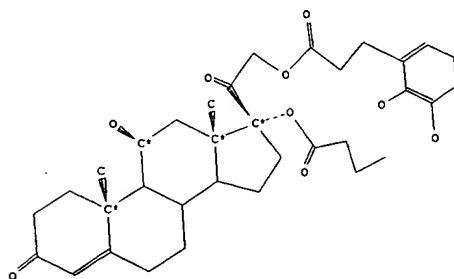


## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1

## L11 ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2931827  
 Beilstein Pref. RN (BPR): 49756-90-3  
 CAS Reg. No. (RN): 49756-90-3  
 Chemical Name (CN): Hydrocortison-17-butytrat-21-<.beta.->(2,3-dihydroxyphenyl)-propionat  
 Autonom Name (AUN): butyric acid 17-<<3-(2,3-dihydroxyphenyl)-propionyloxy>-acetyl>-11-hydroxy-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta<a>phenanthren-17-yl ester  
 Molec. Formula (MF): C34 H44 O9  
 Molecular Weight (MW): 596.72  
 Lawson Number (LN): 12033, 10058, 1173  
 File Segment (FS): Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 2718468  
 Tautomer ID (TAUTID): 2888417  
 Beilstein Citation (BSO): 5-10  
 Entry Date (DED): 1989/07/11  
 Update Date (DUPD): 1989/07/26



## Field Availability:

Code	Name	Occurrence
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BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1

## L11 ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN (Continued)

Code	Name	Occurrence
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1

## This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

## Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

181 - 184 11

## Reference(s):

1. Patent: Dermal Lab. Ltd. DE 2204366 1973, Chem.Abstr., 79(115784)

## Reaction:

RX  
 Reaction ID (.ID): 7872465  
 Product BRN (.PBRN): 2932013  
 Product (.PRO): Hydrocortison-17-valerat-21-<.beta.->(2,3-dihydroxyphenyl)-propionat  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX  
 Reaction RID (.RID): 7872465.1  
 Reaction Classification (.CL): Preparation (half reaction)  
 Reference(s):  
 1. Patent: Dermal Lab. Ltd. DE 2204366 1973, Chem.Abstr., 79(115784)

## L11 ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN (Continued)

Code	Name	Occurrence
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1

## This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

## Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

160 - 165 11

## Reference(s):

1. Patent: Dermal Lab. Ltd. DE 2204366 1973, Chem.Abstr., 79(115784)

## Reaction:

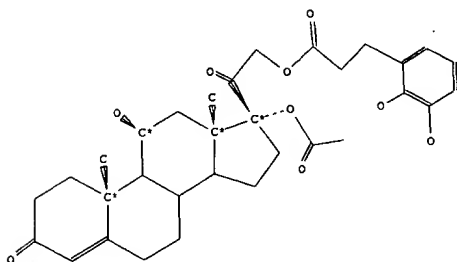
RX  
 Reaction ID (.ID): 7872348  
 Product BRN (.PBRN): 2931827  
 Product (.PRO): Hydrocortison-17-butytrat-21-<.beta.->(2,3-dihydroxyphenyl)-propionat  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX  
 Reaction RID (.RID): 7872348.1  
 Reaction Classification (.CL): Preparation (half reaction)  
 Reference(s):  
 1. Patent: Dermal Lab. Ltd. DE 2204366 1973, Chem.Abstr., 79(115784)

L11 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2931194  
 Beilstein Pref. RN (BPR): 49756-91-4  
 CAS Reg. No. (RN): 49756-91-4  
 Chemical Name (CN): Hydrocortison-17-acetat-21-<.beta.->(2.3-dihydroxyphenyl)-propionat>  
 Autonom Name (AUN): 3-(2,3-dihydroxy-phenyl)-propionic acid  
 2-(17-acetoxy-11-hydroxy-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester  
 C32 H40 O9  
 Molec. Formula (MF): 568.66  
 Molecular Weight (MW): 12033, 10058, 1155  
 Lawson Number (LN): 2717669  
 File Segment (FS): Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 2888356  
 Tautomer ID (TAUTID): 5-10  
 Beilstein Citation (BSO): 1989/07/11  
 Entry Date (DED): 1989/07/26  
 Update Date (DUPD): 1989/07/26



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1

L11 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

(Continued)

Code	Name	Occurrence
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

## Melting Point:

Value	[Ref.]
(MP)	1
(Cel)	1

164 - 166 [1]

## Reference(s):

1. Patent: Dermal Lab. Ltd. DE 2204366 1973, Chem.Abstr., 79(115784)

## Reaction:

RX  
 Reaction ID (.ID): 7871932  
 Product BRN (.PBRN): 2931194  
 Product (.PRO): Hydrocortison-17-acetat-21-<.beta.->(2.3-dihydroxyphenyl)-propionat>  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX  
 Reaction RID (.RID): 7871932.1  
 Reaction Classification (.CL): Preparation (half reaction)  
 Reference(s):  
 1. Patent: Dermal Lab. Ltd. DE 2204366 1973, Chem.Abstr., 79(115784)



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Page 9

=> d ibib ab fqhit 1-3

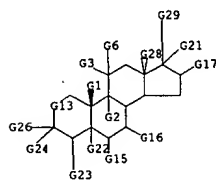
L13 ANSWER 1 OF 3 MARPAT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 136:391016 MARPAT  
 TITLE: Angiostatic agents combined with other agents for lowering and controlling intraocular pressure  
 Clark, Abbot F.  
 INVENTOR(S):  
 PATENT ASSIGNEE(S): Alcon Laboratories, Inc., USA  
 SOURCE: PCT Int. Appl., 19 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040030	A1	20020523	WO 2000-US31557	20001116
WO 2002040030	C1	20021107		
V: AU, BR, CA, CN, JP, MX, PL, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
AU 2001017709	A5	20020527	AU 2001-17709	20001116
EP 1341541	A1	20030910	EP 2000-980450	20001116
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: WO 2000-US31557 20001116  
 AB Angiostatic agents and another IOP lowering compd. are combined in ophthalmic compns. to treat glaucoma and ocular hypertension. Methods for treating glaucoma and ocular hypertension are also disclosed.

MSTR 1A



G1 = Me  
 G5 = cycloalkyl<(3-6)> / alkyl<(1-)> (SR (1-) Ph)  
 G13 = 46



G21 = 83

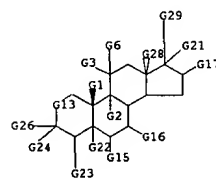
L13 ANSWER 2 OF 3 MARPAT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 134:91141 MARPAT  
 TITLE: Combination therapy for lowering and controlling intraocular pressure containing angiostatic steroids  
 Clark, Abbot F.  
 INVENTOR(S):  
 PATENT ASSIGNEE(S): Alcon Laboratories, Inc., USA  
 SOURCE: U.S., 7 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6172054	B1	20010109	US 1995-491005	19950615
			US 1995-491005	19950615

PRIORITY APPLN. INFO.:  
 AB Angiostatic agents and another IOP lowering compd. are combined in ophthalmic compns. to treat glaucoma and ocular hypertension. Methods for treating glaucoma and ocular hypertension are also disclosed. A soln. was prepd. contg timolol maleate and 4,9(11)-pregnadiene-17.alpha.,21-diol-3,20-dione 21 acetate.

MSTR 1A



G1 = Me  
 G5 = cycloalkyl<(3-6)> / alkyl<(1-)> (SR (1-) Ph)  
 G13 = 46



G21 = 83

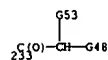


G28 = Me  
 G29 = 233

L13 ANSWER 1 OF 3 MARPAT COPYRIGHT 2004 ACS on STN (Continued)



G28 = Me  
 G29 = 233



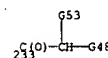
G48 = 207



G24+G26= O  
 MPL: claim 2  
 NTE: and pharmaceutically acceptable salts  
 NTE: additional double bond, oxo, epoxy and methylene formation also claimed  
 NTE: substitution is restricted

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 3 MARPAT COPYRIGHT 2004 ACS on STN (Continued)



G48 = 207



G24+G26= O  
 MPL: claim 1  
 NTE: and pharmaceutically acceptable salts  
 NTE: additional double bond, oxo, epoxy and methylene formation also claimed  
 NTE: substitution is restricted

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 3 MARPAT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 128:294939 MARPAT  
 TITLE: Preparation of nitrate esters of corticoid compounds  
 and pharmaceutical applications thereof  
 Del Soldato, Piero  
 INVENTOR(S): Nicox S.A., Fr.: Del Soldato, Piero  
 PATENT ASSIGNEE(S): PCT Int. Appl., 38 pp.  
 SOURCE: CODEN: P1XXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

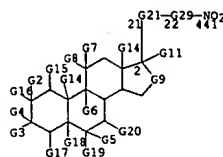
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9815568	A2	19980416	WO 1997-EP5426	19971002
WO 9815568	A3	19980618		
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SE, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9747803	A1	19980505	AU 1997-47803	19971002
AU 719250	B2	20000504		
EP 929565	A2	19990721	EP 1997-910409	19971002
EP 929565	B1	20020529		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, SI, LT, FI, RO				
BR 9711586	A	19990824	BR 1997-11586	19971002
CN 1253563	A	20000517	CN 1997-180284	19971002
JP 2001501637	T2	20010206	JP 1998-517154	19971002
AT 218142	E	20020615	AT 1997-910409	19971002
RU 2186781	C2	20020810	RU 1999-108661	19971002
PT 929565	T	20021031	PT 1997-97910409	19971002
ES 2177952	T3	20021216	ES 1997-910409	19971002
US 6610676	B1	20030826	US 1999-269729	19990402
KR 2000048911	A	20000725	KR 1999-702942	19990403
PRIORITY APPLN. INFO.:				
			IT 1996-M12048	19961004
			WO 1997-EP5426	19971002

AB The title compds. of the general formula B-X1-NO2 or their esters or salts, where B has structure I where there may be substituents in place of the H in the CH group or two hydrogens H2 in the CH2 group shown in the general formula; R and R1 are equal or different one from the other and may be hydrogen or linear or branched alkyls having from 1 to 4 carbon atoms, preferably R = R1 = CH3; B being a corticosteroid residue; R2 is -(CO-L)<sub>x</sub>-(X)<sub>y</sub>- where x and y are integers equal or different one from the other and equal to 0 or 1; where L is a bivalent connecting group; X is equal to X2 where X2 = O, NH, NR3 where R3 is a linear or branched alkyl having from 1 to 10 C atoms; or equal to X3 where X3 is equal to OH, CH3, Cl, N(CH2CH3)2, SCH2F, SH; X1 is a bivalent connecting bridge Y0 where Y is a C1-C20 alkylene were prepd. Thus, hydrocortisone was treated with 4-chlorobutanoyl chloride followed by treatment with AgNO2 to give the nitro deriv. II. II had a 62% antiarthritic activity in rats at 10 mg/kg, but did not affect cardiovascular parameters.

MSTR 1

L13 ANSWER 3 OF 3 MARPAT COPYRIGHT 2004 ACS on STN

(Continued)



G9 = 259

HC-G10  
259

G11 = OCOMe

G14 = Me

G21 = 378-2 381-22

378(O)-CH2-O-381(O)

G31 = phenylene

G32 = alkylene-EC (1-3) C, DC (0) M3&gt;

G3 + G4 = O

DER: or esters or salts

MPL: claim 1

NTE: additional ring fusion also claimed

=> d his

(FILE 'HOME' ENTERED AT 12:04:52 ON 01 MAR 2004)

FILE 'REGISTRY' ENTERED AT 12:05:08 ON 01 MAR 2004

L1 STRUCTURE UPLOADED

L2 5 S L1

L3 118 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:06:11 ON 01 MAR 2004

L4 142 S L3

L5 70 S L4 NOT PY>=1992

FILE 'REGISTRY' ENTERED AT 12:08:51 ON 01 MAR 2004

L6 STRUCTURE UPLOADED

L7 57 S L6 FULL SUB=L3

L8 STRUCTURE UPLOADED

L9 30 S L8 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 12:10:47 ON 01 MAR 2004

L10 2 S L9

FILE 'BEILSTEIN' ENTERED AT 12:13:37 ON 01 MAR 2004

L11 3 S L9 FULL

FILE 'MARPAT' ENTERED AT 12:14:58 ON 01 MAR 2004

L12 4 S L9 FULL

L13 3 S L12 NOT L10